

What is Claimed is:

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1. A computerized method of determining parameters for chemical synthesis comprising:
 - accepting a user identification of a target chemical; and
 - displaying a listing of reagent chemicals that are used to synthesize the target
- 5 chemical, a listing of equipment that is used to synthesize the target chemical and a listing of a procedure that is used to synthesize the target chemical by reacting the reagent chemicals in the equipment according to the procedure, in response to the user identification of the target chemical.
2. A method according to Claim 1 further comprising:
 - accepting user input to order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical; and
- 5 electronically ordering the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical, in response to the user input to order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical.
3. A method according to Claim 1 wherein the accepting a user identification of a target chemical is preceded by:
 - entering into a database, a plurality of target chemicals, a plurality of corresponding listings of reagent chemicals that are used to synthesize the plurality of
- 5 target chemicals, a plurality of corresponding listings of equipment that is used to synthesize the plurality of target chemicals and a plurality of corresponding listings of procedures that are used to synthesize the plurality of target chemicals by reacting the corresponding reagent chemicals in the corresponding equipment according to the corresponding procedure.
4. A method according to Claim 3 further comprising:
 - accepting user input to order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical; and

5 electronically ordering the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical, in response to the user input to order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical.

5. A method according to Claim 1 wherein the accepting a user identification of a target chemical comprises accepting a user identification of a target chemical by chemical formula, chemical structure, chemical compound name and/or CAS number.

5 6. A method according to Claim 1 wherein the accepting a user identification of a target chemical comprises:
displaying a listing of target chemicals that match the user query; and
accepting a user selection of a target chemical from the listing of target
5 chemicals that match the user query.

7. A method according to Claim 1 wherein the accepting a user identification of a target chemical comprises:
accepting a user identification of a reaction type;
displaying a listing of target chemicals that are synthesized using the reaction
5 type; and
accepting a user selection of a target chemical from the listing of target chemicals that are synthesized using the reaction type.

8. A method according to Claim 1 wherein the following is performed between the accepting and the displaying:
displaying a listing of procedures that can be used to synthesize the target
chemical; and
5 accepting a user selection of a procedure from the listing of procedures that can be used to synthesize the target chemical.

9. A method according to Claim 1 wherein the following is performed between the accepting and the displaying:

accepting a user selection of a desired quantity of the target chemical; and
scaling the listing of the reagent chemicals so as to synthesize the desired
5 quantity of the target chemical; and

wherein the displaying comprises:

displaying a scaled listing of the reagent chemicals that are used to synthesize
the desired quantity of the target chemical, a listing of equipment that is used to
synthesize the desired quantity of the target chemical and a listing of a procedure that
10 is used to synthesize the desired quantity of the target chemical by reacting the
reagent chemicals in the equipment according to the procedure, in response to the user
identification of the target chemical and the user selection of the desired quantity of
the target chemical.

10. A method according to Claim 1 wherein the accepting a user
identification of a target chemical comprises:

displaying a prioritized listing of target chemicals that match the user query;
and

5 accepting a user selection of a target chemical from the prioritized listing of
target chemicals that match the user query.

11. A method according to Claim 1 wherein the accepting a user
identification of a target chemical comprises:

accepting user identification of a chemical;

displaying a listing of procedures that use the chemical as a reagent chemical;

5 and

accepting a user selection of a procedure from the listing of procedures that
use the chemical as a reagent chemical.

12. A computerized method of determining parameters for chemical
synthesis comprising:

entering into a database, a plurality of target chemicals, a plurality of
corresponding listings of reagent chemicals that are used to synthesize the plurality of
5 target chemicals, a plurality of corresponding listings of equipment that is used to
synthesize the plurality of target chemicals and a plurality of corresponding listings of
procedures that are used to synthesize the plurality of target chemicals by reacting the

corresponding reagent chemicals in the corresponding equipment according to the corresponding procedure.

13. A method according to Claim 12 further comprising:

accepting user input to order one of the target chemicals, reagent chemicals that are used to synthesize the one of the target chemicals and/or equipment that is used to synthesize the one of the target chemicals; and

5 electronically ordering the one of the target chemicals, the reagent chemicals that are used to synthesize the one of the target chemicals and/or the equipment that is used to synthesize the one of the target chemicals, in response to the user input to order the one of the target chemicals, the reagent chemicals that are used to synthesize the one of the target chemicals and/or the equipment that is used to synthesize the one
10 of the target chemicals.

14. A method according to Claim 12 wherein the entering comprises interactively entering into the database a narrative description of steps of the corresponding procedure using the corresponding listing of the reagent chemicals and the corresponding listing of the equipment.

15. A method according to Claim 12 wherein the entering comprises accepting user entry of a listing of reagent chemicals that are used in a next step of a procedure to synthesize a target chemical, user entry of a listing of corresponding equipment that is used in the next step of the procedure to synthesize the target
5 chemical and user entry of the next step of the procedure to synthesize the target chemical, in response to user indication that the next step is present in the procedure.

16. A method according to Claim 12 wherein the entering is preceded by identifying a target chemical, reagent chemicals that are used to synthesize the target chemical, equipment that is used to synthesize the target chemical and a procedure that is used to synthesize the target chemical by reacting the reagent chemicals in the
5 equipment according to the procedure, from a publication related to synthesis of the target chemical and/or from proprietary data related to synthesis of the target chemical.

17. A method according to Claim 12 wherein the entering comprises:
entering into a chemical database, a plurality of target chemicals, a plurality of
first pointers to a corresponding plurality of listings of reagent chemicals in the
chemical database that are used to synthesize the plurality of target chemicals, a
5 plurality of second pointers to a corresponding plurality of listings of equipment in an
equipment database that is used to synthesize the plurality of target chemicals, and a
plurality of corresponding listings of procedures that are used to synthesize the
plurality of target chemicals by reacting the corresponding reagent chemicals in the
corresponding equipment according to the corresponding procedure; and
10 entering into the equipment database, the plurality of listings of equipment that
is used to synthesize the plurality of target chemicals.

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18. A computerized method of obtaining materials for chemical synthesis
comprising:

electronically ordering a target chemical, reagent chemicals that are used to
synthesize the target chemical and/or equipment that is used to synthesize the target
5 chemical, from an electronically displayed listing of the reagent chemicals that are
used to synthesize the target chemical, of the equipment that is used to synthesize the
target chemical and of a procedure that is used to synthesize the target chemical by
reacting the reagent chemicals in the equipment according to the procedure, in
response to user input to order the target chemical, the reagent chemicals that are used
10 to synthesize the target chemical and/or the equipment that is used to synthesize the
target chemical.

19. A method according to Claim 18 wherein the electronically ordering
comprises:

electronically ordering a kit of the reagent chemicals that are used to
synthesize the target chemical.

20. A method according to Claim 18 wherein the electronically ordering
comprises:

electronically ordering a kit of the equipment that is used to synthesize the
target chemical.

25. A system according to Claim 24 further comprising:

means for accepting user input to order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical; and

5 means for electronically ordering the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical, in response to the user input to order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical.

26. A system according to Claim 24 further comprising:

a database; and

5 means for entering into the database, a plurality of target chemicals, a plurality of corresponding listings of reagent chemicals that are used to synthesize the plurality of target chemicals, a plurality of corresponding listings of equipment that is used to synthesize the plurality of target chemicals and a plurality of corresponding listings of procedures that are used to synthesize the plurality of target chemicals by reacting the corresponding reagent chemicals in the corresponding equipment according to the corresponding procedure.

27. A system according to Claim 26 further comprising:

means for accepting user input to order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical; and

5 means for electronically ordering the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical, in response to the user input to order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical.

28. A system according to Claim 24 wherein the means for accepting a user identification of a target chemical comprises means for accepting a user identification of a target chemical by chemical formula, chemical structure, chemical compound name and/or CAS number.

29. A system according to Claim 24 wherein the means for accepting a user identification of a target chemical comprises:

means for displaying a listing of target chemicals that match the user query;
and

5 means for accepting a user selection of a target chemical from the listing of target chemicals that match the user query.

30. A system according to Claim 24 wherein the means for accepting a user identification of a target chemical comprises:

means for accepting a user identification of a reaction type;

5 means for displaying a listing of target chemicals that are synthesized using the reaction type; and

means for accepting a user selection of a target chemical from the listing of target chemicals that are synthesized using the reaction type.

31. A system according to Claim 24 further comprising:

means for displaying a listing of procedures that can be used to synthesize the target chemical; and

5 means for accepting a user selection of a procedure from the listing of procedures that can be used to synthesize the target chemical.

32. A system according to Claim 24 further comprising:

means for accepting a user selection of a desired quantity of the target chemical; and

5 means for scaling the listing of the reagent chemicals so as to synthesize the desired quantity of the target chemical; and

wherein the means for displaying comprises:

10 means for displaying a scaled listing of the reagent chemicals that are used to synthesize the desired quantity of the target chemical, a listing of equipment that is used to synthesize the desired quantity of the target chemical and a listing of a procedure that is used to synthesize the desired quantity of the target chemical by reacting the reagent chemicals in the equipment according to the procedure, in

response to the user identification of the target chemical and the user selection of the desired quantity of the target chemical.

33. A system according to Claim 24 wherein the means for accepting a user identification of a target chemical comprises:

means for displaying a prioritized listing of target chemicals that match the user query; and

5 means for accepting a user selection of a target chemical from the prioritized listing of target chemicals that match the user query.

34. A system according to Claim 24 wherein the means for accepting a user identification of a target chemical comprises:

means for accepting user identification of a chemical;

5 means for displaying a listing of procedures that use the chemical as a reagent chemical; and

means for accepting a user selection of a procedure from the listing of procedures that use the chemical as a reagent chemical.

35. A system for determining parameters for chemical synthesis comprising:

a database; and

5 means for entering into the database, a plurality of target chemicals, a plurality of corresponding listings of reagent chemicals that are used to synthesize the plurality of target chemicals, a plurality of corresponding listings of equipment that is used to synthesize the plurality of target chemicals and a plurality of corresponding listings of procedures that are used to synthesize the plurality of target chemicals by reacting the corresponding reagent chemicals in the corresponding equipment according to the
10 corresponding procedure.

36. A system according to Claim 35 further comprising:

means for accepting user input to order one of the target chemicals, reagent chemicals that are used to synthesize the one of the target chemicals and/or equipment that is used to synthesize the one of the target chemicals; and

5 means for electronically ordering the one of the target chemicals, the reagent
chemicals that are used to synthesize the one of the target chemicals and/or the
equipment that is used to synthesize the one of the target chemicals, in response to the
user input to order the one of the target chemicals, the reagent chemicals that are used
to synthesize the one of the target chemicals and/or the equipment that is used to
10 synthesize the one of the target chemicals.

37. A system according to Claim 35 wherein the means for entering
comprises means for interactively entering into the database a narrative description of
steps of the corresponding procedure using the corresponding listing of the reagent
chemicals and the corresponding listing of the equipment.

38. A system according to Claim 35 wherein the means for entering
comprises means for accepting user entry of a listing of reagent chemicals that are
used in a next step of a procedure to synthesize a target chemical, user entry of a
listing of corresponding equipment that is used in the next step of the procedure to
5 synthesize the target chemical and user entry of the next step of the procedure to
synthesize the target chemical, in response to user indication that the next step is
present in the procedure.

39. A system according to Claim 35 further comprising means for
identifying a target chemical, reagent chemicals that are used to synthesize the target
chemical, equipment that is used to synthesize the target chemical and a procedure
that is used to synthesize the target chemical by reacting the reagent chemicals in the
5 equipment according to the procedure, from a publication related to synthesis of the
target chemical and/or from proprietary data related to synthesis of the target
chemical.

40. A system according to Claim 35 wherein the database comprises a
chemical database and an equipment database, and the means for entering comprises:
means for entering into the chemical database, a plurality of target chemicals,
a plurality of first pointers to a corresponding plurality of listings of reagent chemicals
5 in the chemical database that are used to synthesize the plurality of target chemicals, a
plurality of second pointers to a corresponding plurality of listings of equipment in the

equipment database that is used to synthesize the plurality of target chemicals, and a plurality of corresponding listings of procedures that are used to synthesize the plurality of target chemicals by reacting the corresponding reagent chemicals in the
10 corresponding equipment according to the corresponding procedure; and

means for entering into the equipment database, the plurality of listings of equipment that is used to synthesize the plurality of target chemicals.

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41. A system for obtaining materials for chemical synthesis comprising:
an electronically displayed listing of reagent chemicals that are used to synthesize a target chemical, of equipment that is used to synthesize the target chemical and of a procedure that is used to synthesize the target chemical by reacting
5 the reagent chemicals in the equipment according to the procedure; and

means for electronically ordering the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical, from the electronically displayed listing of the reagent chemicals that are used to synthesize the target chemical, of the equipment that is
10 used to synthesize the target chemical and of the procedure that is used to synthesize the target chemical by reacting the reagent chemicals in the equipment according to the procedure, in response to user input to order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical.

42. A system according to Claim 41 wherein the means for electronically ordering comprises:

means for electronically ordering a kit of the reagent chemicals that are used to synthesize the target chemical.

43. A system according to Claim 41 wherein the means for electronically ordering comprises:

means for electronically ordering a kit of the equipment that is used to synthesize the target chemical.

44. A computer program product that determines parameters for chemical synthesis, the computer program product comprising a computer usable storage

medium having computer-readable program code embodied in the medium, the computer-readable program code comprising:

5 computer-readable program code that is configured to accept a user identification of a target chemical; and

computer-readable program code that is configured to display a listing of reagent chemicals that are used to synthesize the target chemical, a listing of equipment that is used to synthesize the target chemical and a listing of a procedure
10 that is used to synthesize the target chemical by reacting the reagent chemicals in the equipment according to the procedure, in response to the user identification of the target chemical.

45. A computer program product according to Claim 44 further comprising:

computer-readable program code that is configured to accept user input to order the target chemical, the reagent chemicals that are used to synthesize the target
5 chemical and/or the equipment that is used to synthesize the target chemical; and

computer-readable program code that is configured to electronically order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical, in response to the user input to order the target chemical, the reagent chemicals that are used to
10 synthesize the target chemical and/or the equipment that is used to synthesize the target chemical.

46. A computer program product according to Claim 44 further comprising:

computer-readable program code that is configured to enter into a database, a plurality of target chemicals, a plurality of corresponding listings of reagent chemicals
5 that are used to synthesize the plurality of target chemicals, a plurality of corresponding listings of equipment that is used to synthesize the plurality of target chemicals and a plurality of corresponding listings of procedures that are used to synthesize the plurality of target chemicals by reacting the corresponding reagent chemicals in the corresponding equipment according to the corresponding procedure.

47. A computer program product according to Claim 46 further comprising:

computer-readable program code that is configured to accept user input to order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical; and

computer-readable program code that is configured to electronically order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical, in response to the user input to order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical.

48. A computer program product according to Claim 44 wherein the computer-readable program code that is configured to accept a user identification of a target chemical comprises computer-readable program code that is configured to accept a user identification of a target chemical by chemical formula, chemical structure, chemical compound name and/or CAS number.

49. A computer program product according to Claim 44 wherein the computer-readable program code that is configured to accept a user identification of a target chemical comprises:

computer-readable program code that is configured to display a listing of target chemicals that match the user query; and

computer-readable program code that is configured to accept a user selection of a target chemical from the listing of target chemicals that match the user query.

50. A computer program product according to Claim 44 wherein the computer-readable program code that is configured to accept a user identification of a target chemical comprises:

computer-readable program code that is configured to accept a user identification of a reaction type;

computer-readable program code that is configured to display a listing of target chemicals that are synthesized using the reaction type; and

computer-readable program code that is configured to accept a user selection of a target chemical from the listing of target chemicals that are synthesized using the reaction type.

51. A computer program product according to Claim 44 further comprising:

computer-readable program code that is configured to display a listing of procedures that can be used to synthesize the target chemical; and

5 computer-readable program code that is configured to accept a user selection of a procedure from the listing of procedures that can be used to synthesize the target chemical.

52. A computer program product according to Claim 44 further comprising:

computer-readable program code that is configured to accept a user selection of a desired quantity of the target chemical; and

5 computer-readable program code that is configured to scale the listing of the reagent chemicals so as to synthesize the desired quantity of the target chemical; and

wherein the computer-readable program code that is configured to display comprises:

10 computer-readable program code that is configured to display a scaled listing of the reagent chemicals that are used to synthesize the desired quantity of the target chemical, a listing of equipment that is used to synthesize the desired quantity of the target chemical and a listing of a procedure that is used to synthesize the desired quantity of the target chemical by reacting the reagent chemicals in the equipment according to the procedure, in response to the user identification of the target
15 chemical and the user selection of the desired quantity of the target chemical.

53. A computer program product according to Claim 44 wherein the computer-readable program code that is configured to accept a user identification of a target chemical comprises:

5 computer-readable program code that is configured to display a prioritized listing of target chemicals that match the user query; and

computer-readable program code that is configured to accept a user selection of a target chemical from the prioritized listing of target chemicals that match the user query.

54. A computer program product according to Claim 44 wherein the computer-readable program code that is configured to accept a user identification of a target chemical comprises:

5 computer-readable program code that is configured to accept user identification of a chemical;

computer-readable program code that is configured to display a listing of procedures that use the chemical as a reagent chemical; and

10 computer-readable program code that is configured to accept a user selection of a procedure from the listing of procedures that use the chemical as a reagent chemical.

55. A computer program product that determines parameters for chemical synthesis, the computer program product comprising a computer usable storage medium having computer-readable program code embodied in the medium, the computer-readable program code comprising:

5 computer-readable program code that is configured to enter into a database, a plurality of target chemicals, a plurality of corresponding listings of reagent chemicals that are used to synthesize the plurality of target chemicals, a plurality of corresponding listings of equipment that is used to synthesize the plurality of target chemicals and a plurality of corresponding listings of procedures that are used to
10 synthesize the plurality of target chemicals by reacting the corresponding reagent chemicals in the corresponding equipment according to the corresponding procedure.

56. A computer program product according to Claim 55 further comprising:

5 computer-readable program code that is configured to accept user input to order one of the target chemicals, reagent chemicals that are used to synthesize the one of the target chemicals and/or equipment that is used to synthesize the one of the target chemicals; and

computer-readable program code that is configured to electronically order the one of the target chemicals, the reagent chemicals that are used to synthesize the one of the target chemicals and/or the equipment that is used to synthesize the one of the target chemicals, in response to the user input to order the one of the target chemicals, the reagent chemicals that are used to synthesize the one of the target chemicals and/or the equipment that is used to synthesize the one of the target chemicals.

57. A computer program product according to Claim 55 wherein the computer-readable program code that is configured to enter comprises computer-readable program code that is configured to interactively enter into the database a narrative description of steps of the corresponding procedure using the corresponding listing of the reagent chemicals and the corresponding listing of the equipment.

58. A computer program product according to Claim 55 wherein the computer-readable program code that is configured to enter comprises computer-readable program code that is configured to accept user entry of a listing of reagent chemicals that are used in a next step of a procedure to synthesize a target chemical, user entry of a listing of corresponding equipment that is used in the next step of the procedure to synthesize the target chemical and user entry of the next step of the procedure to synthesize the target chemical, in response to user indication that the next step is present in the procedure.

59. A computer program product according to Claim 55 further comprising:

computer-readable program code that is configured to identify a target chemical, reagent chemicals that are used to synthesize the target chemical, equipment that is used to synthesize the target chemical and a procedure that is used to synthesize the target chemical by reacting the reagent chemicals in the equipment according to the procedure, from a publication related to synthesis of the target chemical and/or from proprietary data related to synthesis of the target chemical.

60. A method according to Claim 55 wherein the computer-readable program code that is configured to enter comprises:

computer-readable program code that is configured to enter into a chemical database, a plurality of target chemicals, a plurality of first pointers to a corresponding
5 plurality of listings of reagent chemicals in the chemical database that are used to synthesize the plurality of target chemicals, a plurality of second pointers to a corresponding plurality of listings of equipment in an equipment database that is used to synthesize the plurality of target chemicals, and a plurality of corresponding listings of procedures that are used to synthesize the plurality of target chemicals by
10 reacting the corresponding reagent chemicals in the corresponding equipment according to the corresponding procedure; and

computer-readable program code that is configured to enter into the equipment database, the plurality of listings of equipment that is used to synthesize the plurality of target chemicals.

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61. A computer program product that obtains materials for chemical synthesis, the computer program product comprising a computer usable storage medium having computer-readable program code embodied in the medium, the computer-readable program code comprising:

5 computer-readable program code that is configured to electronically order a target chemical, reagent chemicals that are used to synthesize the target chemical and/or equipment that is used to synthesize the target chemical, from an electronically displayed listing of the reagent chemicals that are used to synthesize the target chemical, of the equipment that is used to synthesize the target chemical and of a
10 procedure that is used to synthesize the target chemical by reacting the reagent chemicals in the equipment according to the procedure, in response to user input to order the target chemical, the reagent chemicals that are used to synthesize the target chemical and/or the equipment that is used to synthesize the target chemical.

62. A computer program product according to Claim 61 wherein the computer-readable program code that is configured to electronically order comprises:

computer-readable program code that is configured to electronically order a kit of the reagent chemicals that are used to synthesize the target chemical.

63. A computer program product according to Claim 61 wherein the computer-readable program code that is configured to electronically order comprises:

computer-readable program code that is configured to electronically order a kit of the equipment that is used to synthesize the target chemical.

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